

FILE 'REGISTRY' ENTERED AT 14:14:21 ON 27 AUG 2007

~~L14 177404 S N2CSC/ES~~

~~L15 STRUCTURE UPLOADED~~

L16 50 S L15 SAM SUB=L14

FILE 'STNGUIDE' ENTERED AT 14:15:40 ON 27 AUG 2007

FILE 'REGISTRY' ENTERED AT 14:26:43 ON 27 AUG 2007

~~L17 5390 S L15 SSS FULL SUB=L14~~

FILE 'STNGUIDE' ENTERED AT 14:26:58 ON 27 AUG 2007

FILE 'REGISTRY' ENTERED AT 14:28:07 ON 27 AUG 2007

~~L18 STRUCTURE UPLOADED~~

L19 50 S L18 SAM SUB=L17

~~L20 4309 S L18 SSS FULL SUB=L17~~

FILE 'CAPLUS' ENTERED AT 14:29:07 ON 27 AUG 2007

L21 783 S L20

FILE 'STNGUIDE' ENTERED AT 14:29:42 ON 27 AUG 2007

FILE 'REGISTRY' ENTERED AT 14:30:19 ON 27 AUG 2007

FILE 'CAPLUS' ENTERED AT 14:30:27 ON 27 AUG 2007

FILE 'REGISTRY' ENTERED AT 14:30:27 ON 27 AUG 2007

FILE 'CAPLUS' ENTERED AT 14:30:32 ON 27 AUG 2007

FILE 'STNGUIDE' ENTERED AT 14:30:50 ON 27 AUG 2007

FILE 'REGISTRY' ENTERED AT 14:31:22 ON 27 AUG 2007

~~L22 STRUCTURE UPLOADED~~

L23 50 S L22 SAM SUB=L20

~~L24 990 S L22 SSS FULL SUB=L20~~

~~L25 3319 S L20 NOT L24~~

FILE 'CAPLUS' ENTERED AT 14:32:01 ON 27 AUG 2007

L26 545 S L25

FILE 'CAPLUS' ENTERED AT 14:32:49 ON 27 AUG 2007

FILE 'STNGUIDE' ENTERED AT 14:33:20 ON 27 AUG 2007

FILE 'CAPLUS' ENTERED AT 14:33:32 ON 27 AUG 2007

FILE 'STNGUIDE' ENTERED AT 14:34:21 ON 27 AUG 2007

FILE 'REGISTRY' ENTERED AT 14:40:59 ON 27 AUG 2007

~~SAV TEM L25 BRD 575093/A~~

~~L27 STRUCTURE UPLOADED~~

L28 0 S L27 SAM SUB=L25

~~L29 3 S L27 SSS FULL SUB=L25~~

Elected

FILE 'CAPLUS' ENTERED AT 14:43:01 ON 27 AUG 2007

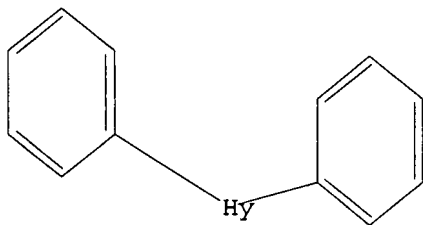
L30 2 S L29

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FILE 'CAPLUS' ENTERED AT 14:44:20 ON 27 AUG 2007

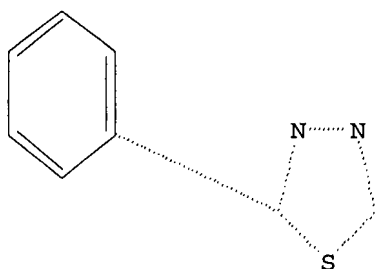
FILE 'REGISTRY' ENTERED AT 14:47:07 ON 27 AUG 2007

=> d 115
L15 HAS NO ANSWERS
L15 STR



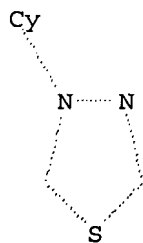
Structure attributes must be viewed using STN Express query preparation.

=> d 118
L18 HAS NO ANSWERS
L18 STR



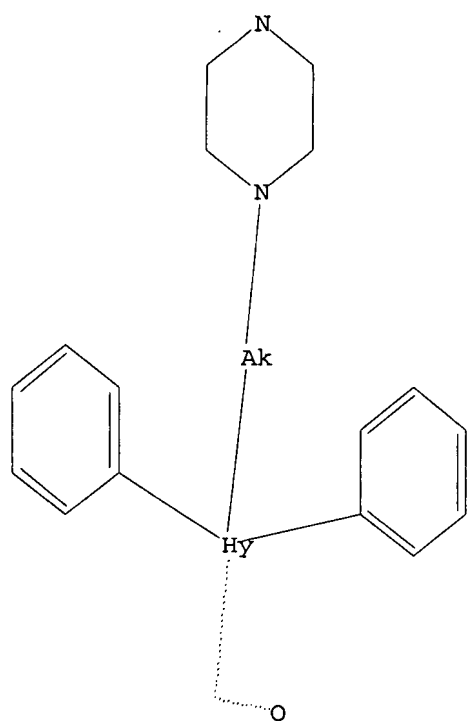
Structure attributes must be viewed using STN Express query preparation.

=> d 122
L22 HAS NO ANSWERS
L22 STR

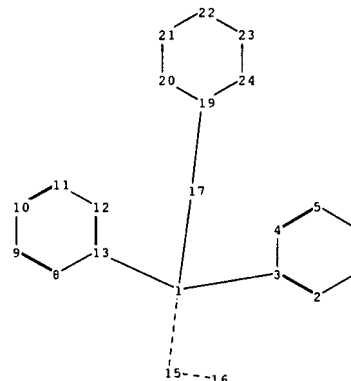
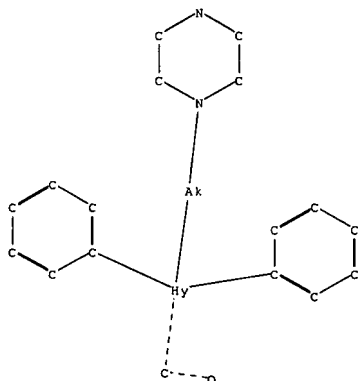


Structure attributes must be viewed using STN Express query preparation.

=> d 127
L27 HAS NO ANSWERS
L27 STR



Structure attributes must be viewed using STN Express query preparation.



chain nodes :

1 15 16 17

ring nodes :

2 3 4 5 6 7 8 9 10 11 12 13 19 20 21 22 23 24

chain bonds :

1-13 1-3 1-15 1-17 15-16 17-19

ring bonds :

2-3 2-7 3-4 4-5 5-6 6-7 8-9 8-13 9-10 10-11 11-12 12-13 19-20 19-24 20-21
21-22 22-23 23-24

exact/norm bonds :

1-13 1-3 1-15 1-17 15-16 17-19 19-20 19-24 20-21 21-22 22-23 23-24

normalized bonds :

2-3 2-7 3-4 4-5 5-6 6-7 8-9 8-13 9-10 10-11 11-12 12-13

isolated ring systems :

containing 2 : 8 : 19 :

Connectivity :

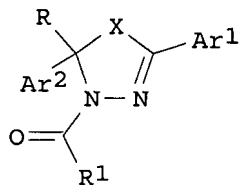
17:2 E exact RC ring/chain

Match level :

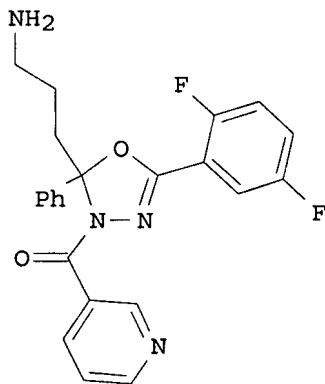
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 15:CLASS 16:CLASS 17:CLASS 19:Atom 20:Atom 21:Atom 22:Atom
23:Atom 24:Atom

AN 2006:383814 CAPLUS
 DN 144:432819
 TI Preparation of oxadiazole and thiadiazole derivatives as mitotic kinesin inhibitors
 IN Hans, Jeremy; Wallace, Eli M.; Zhao, Qian; Lyssikatos, Joseph P.; Aicher, Tom; Laird, Ellen; Robinson, John; Allen, Shelley
 PA Array Biopharma Inc., USA
 SO PCT Int. Appl., 202 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2006044825	A2	20060427	WO 2005-US37305	20051018
	WO 2006044825	A3	20061005		
	W:				
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	RW:				
	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	US 2006100161	A1	20060511	US 2005-252232	20051017
	AU 2005295403	A1	20060427	AU 2005-295403	20051018
	CA 2584866	A1	20060427	CA 2005-2584866	20051018
	EP 1809280	A2	20070725	EP 2005-819172	20051018
	R:				
	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, YU				
PRAI	US 2004-620048P	P	20041019		
	US 2005-252232	A	20051017		
	WO 2005-US37305	W	20051018		
OS	MARPAT 144:432819				
GI					



I



II

AB Oxadiazole and thiadiazole derivs. I, wherein X is O, S; R is ZR₂R₃, Z-OH, Z-substituted phosphate; R₁ is substituted alkyl, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocycloalkyl, OR₃, substituted oxime, acyl,

substituted amine; Ar1 and Ar2 are independently substituted aryl, heteroaryl; R2 is H, acyl, substituted sulfonyl, alkyl, alkenyl, alkynyl, cycloalkyl, amino acid, polypeptide; R3 is H, acyl, alkyl, alkenyl, alkynyl, cycloalkyl; R2 and R3 together with nitrogen to which they are attached form saturated or partially unsatd. heterocycle; Z is substituted alkylene having 1 to 6 carbons, alkenylene or alkynylene each having from 2 to 6 carbons, were prepared as mitotic kinesin inhibitors, particularly kinesin spindle protein (KSP) in the treatment and prevention of hyperproliferative disorders cancer, autoimmune disease, arthritis, graft rejection, inflammatory bowel disease, or proliferation induced after medical procedures. Thus, oxadiazole II was prepared and tested in vitro as mitotic kinesin inhibitor ($IC_{50} < 50 \mu M$). The ability of title compds. to inhibit cellular viability was determined in vitro ($EC_{50} < 50 \mu M$).

IT 885064-26-6P

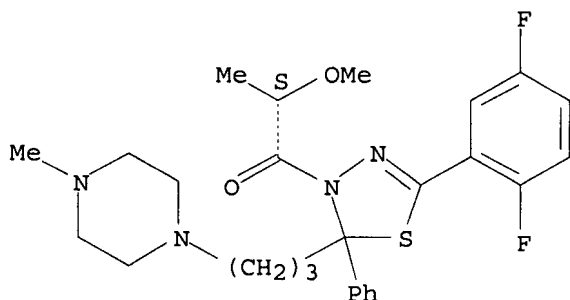
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of oxadiazole and thiadiazole derivs. as mitotic kinesin inhibitors)

RN 885064-26-6 CAPLUS

CN 1,3,4-Thiadiazole, 5-(2,5-difluorophenyl)-2,3-dihydro-3-[(2S)-2-methoxy-1-oxopropyl]-2-[3-(4-methyl-1-piperazinyl)propyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



substituted amine; Ar1 and Ar2 are independently substituted aryl, heteroaryl; R2 is H, acyl, substituted sulfonyl, alkyl, alkenyl, alkynyl, cycloalkyl, amino acid, polypeptide; R3 is H, acyl, alkyl, alkenyl, alkynyl, cycloalkyl; R2 and R3 together with nitrogen to which they are attached form saturated or partially unsatd. heterocycle; Z is substituted alkylene having 1 to 6 carbons, alkenylene or alkynylene each having from 2 to 6 carbons, were prepared as mitotic kinesin inhibitors, particularly kinesin spindle protein (KSP) in the treatment and prevention of hyperproliferative disorders cancer, autoimmune disease, arthritis, graft rejection, inflammatory bowel disease, or proliferation induced after medical procedures. Thus, oxadiazole II was prepared and tested in vitro as mitotic kinesin inhibitor (IC50 < 50 µM). The ability of title compds. to inhibit cellular viability was determined in vitro (EC50 < 50 µM).

~~130~~ ~~ANSWER-2-OF-2~~ ~~CAPLUS~~ ~~COPYRIGHT-2007-ACS-on-STN~~

AN 2005:346997 CAPLUS

DN 142:411362

TI Preparation of thiadiazoline derivatives as M-phase kinesin Eg5 inhibitors for treatment of tumor

IN Murakata, Chikara; Amishiro, Nobuyoshi; Ino, Yoji; Yamamoto, Junichiro; Atsumi, Toshiyuki; Nakai, Ryuichiro; Nakano, Tomohisa

PA Kyowa Hakko Kogyo Co., Ltd., Japan; Fuji Photo Film Co., Ltd.

SO PCT Int. Appl., 118 pp.

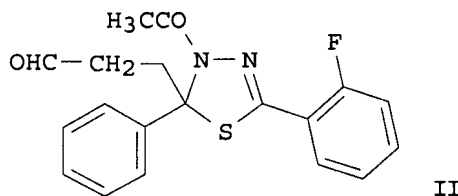
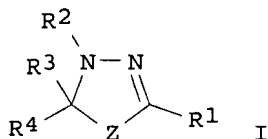
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005035512	A1	20050421	WO 2004-JP15293	20041008
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA 2542034	A1	20050421	CA 2004-2542034	20041008
	EP 1671957	A1	20060621	EP 2004-792510	20041008
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
	US 2007112044	A1	20070517	US 2006-575093	20061207
PRAI	JP 2003-351872	A	20031010		
	JP 2003-360263	A	20031021		
	WO 2004-JP15293	W	20041008		
OS	MARPAT 142:411362				
GI					



AB The title thiadiazoline derivs. I [wherein Z = S or SO; R1 =

(un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, (un)substituted alkyl, etc.; R3 = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, aryl, or heterocyclyl; R4 = (un)substituted alkyl, alkenyl, alkynyl, etc.] or pharmaceutically acceptable salts thereof are prepared as antitumor agents. For example, the compound II was prepared in a multi-step synthesis. II inhibited human tumor cell growth with GI50 of 0.083 μ M.

Formulations containing I as an active ingredient were also described.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT